

E-type delayed fluorescence of a phosphine-
supported $\text{Cu}_2(\mu\text{-NAr}_2)_2$ diamond core:
Harvesting singlet and triplet excitons in OLEDs

Supporting Information^ψ

Joseph C. Deaton^{†*}, Steven C. Switalski[†], Denis Y. Kondakov[†], Ralph H. Young[†],
Thomas D. Pawlik[†], David J. Giesen[†], Seth B. Harkins[‡], Alex J. M. Miller[‡], Seth F.
Mickenberg[‡], Jonas C. Peters^{‡*}

[†]Eastman Kodak Company, Rochester, New York 14650, prior to December, 2009;

[‡]Division of Chemistry and Chemical Engineering, California Institute of Technology,
Pasadena, CA, 91125; [‡]Department of Chemistry, Massachusetts Institute of Technology,
Cambridge, MA, 02139

^ψWork that was carried out at Eastman Kodak Company was done prior to Dec, 2009.

Complete ref. 46:

Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman,
J. R.; Montgomery, J. A.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar,

S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; Pople, J. A. Gaussian 03; Revision B.05 ed.; Gaussian, Inc: Pittsburgh, PA, 2003.

Calculation Details

Ground state geometries were optimized using the Jaguar program with the following keywords:

```
dftname=b3lyp basis=midix igeopt=1 maxitg=30 iacscf=1 maxit=300
```

And the following &atomic block:

```
&atomic
atom basis
CU1 lacv3p
CU2 lacv3p
&
```

The optimized geometry was then used in a single point calculation to obtain the energy and ground state orbitals with the following input file:

```
$gen
dftname=b3lyp basis=midix igeopt=0 maxit=300
cut10=5.0e-4 cut20=5.0e-4 ip1=2 ip102=10
$
$zmat
```

CU1						
CU2	CU1	b2				
P3	CU2	b3	CU1	a3		
P4	CU1	b4	CU2	a4	P3	d4
P5	CU1	b5	CU2	a5	P3	d5
P6	CU2	b6	CU1	a6	P3	d6
C7	P5	b7	CU1	a7	CU2	d7
C8	P5	b8	CU1	a8	CU2	d8
C9	P4	b9	CU1	a9	CU2	d9
C10	P4	b10	CU1	a10	CU2	d10
C11	P6	b11	CU2	a11	CU1	d11
C12	P6	b12	CU2	a12	CU1	d12
C13	P3	b13	CU2	a13	CU1	d13
C14	P3	b14	CU2	a14	CU1	d14
N15	CU2	b15	CU1	a15	P3	d15
N16	CU2	b16	CU1	a16	P3	d16
C17	P6	b17	CU2	a17	CU1	d17
C18	C17	b18	P6	a18	CU2	d18
C19	C18	b19	C17	a19	P6	d19
C20	C19	b20	C18	a20	C17	d20
C21	C20	b21	C19	a21	C18	d21
C22	C21	b22	C20	a22	C19	d22
C23	N16	b23	CU2	a23	CU1	d23
C24	C23	b24	N16	a24	CU2	d24
C25	C24	b25	C23	a25	N16	d25
C26	C25	b26	C24	a26	C23	d26
C27	C26	b27	C25	a27	C24	d27
C28	C27	b28	C26	a28	C25	d28
C29	P3	b29	CU2	a29	CU1	d29
C30	C29	b30	P3	a30	CU2	d30
C31	C30	b31	C29	a31	P3	d31
C32	C31	b32	C30	a32	C29	d32
C33	C32	b33	C31	a33	C30	d33
C34	C33	b34	C32	a34	C31	d34
C35	N15	b35	CU2	a35	CU1	d35
C36	C35	b36	N15	a36	CU2	d36
C37	C36	b37	C35	a37	N15	d37
C38	C37	b38	C36	a38	C35	d38
C39	C38	b39	C37	a39	C36	d39
C40	C39	b40	C38	a40	C37	d40
H41	C7	b41	P5	a41	CU1	d41
H42	C7	b42	P5	a42	CU1	d42
C43	C7	b43	P5	a43	CU1	d43
H44	C8	b44	P5	a44	CU1	d44
H45	C8	b45	P5	a45	CU1	d45
C46	C8	b46	P5	a46	CU1	d46

H47	C9	b47	P4	a47	CU1	d47
C48	C9	b48	P4	a48	CU1	d48
H49	C9	b49	P4	a49	CU1	d49
H50	C10	b50	P4	a50	CU1	d50
C51	C10	b51	P4	a51	CU1	d51
H52	C10	b52	P4	a52	CU1	d52
H53	C11	b53	P6	a53	CU2	d53
H54	C11	b54	P6	a54	CU2	d54
C55	C11	b55	P6	a55	CU2	d55
H56	C12	b56	P6	a56	CU2	d56
H57	C12	b57	P6	a57	CU2	d57
C58	C12	b58	P6	a58	CU2	d58
H59	C13	b59	P3	a59	CU2	d59
C60	C13	b60	P3	a60	CU2	d60
H61	C13	b61	P3	a61	CU2	d61
H62	C14	b62	P3	a62	CU2	d62
C63	C14	b63	P3	a63	CU2	d63
H64	C14	b64	P3	a64	CU2	d64
H65	C18	b65	C17	a65	P6	d65
C66	C19	b66	C18	a66	C17	d66
H67	C20	b67	C19	a67	C18	d67
H68	C21	b68	C20	a68	C19	d68
H69	C24	b69	C23	a69	N16	d69
H70	C25	b70	C24	a70	C23	d70
C71	C26	b71	C25	a71	C24	d71
H72	C27	b72	C26	a72	C25	d72
C73	C29	b73	P3	a73	CU2	d73
H74	C30	b74	C29	a74	P3	d74
H75	C33	b75	C32	a75	C31	d75
H76	C34	b76	C33	a76	C32	d76
H77	C35	b77	N15	a77	CU2	d77
H78	C36	b78	C35	a78	N15	d78
H79	C39	b79	C38	a79	C37	d79
C80	C40	b80	C39	a80	C38	d80
C81	C43	b81	C7	a81	P5	d81
C82	C43	b82	C7	a82	P5	d82
H83	C43	b83	C7	a83	P5	d83
H84	C81	b84	C43	a84	C7	d84
H85	C81	b85	C43	a85	C7	d85
H86	C81	b86	C43	a86	C7	d86
H87	C82	b87	C43	a87	C7	d87
H88	C82	b88	C43	a88	C7	d88
H89	C82	b89	C43	a89	C7	d89
C90	C46	b90	C8	a90	P5	d90
C91	C46	b91	C8	a91	P5	d91
H92	C46	b92	C8	a92	P5	d92

H93	C90	b93	C46	a93	C8	d93
H94	C90	b94	C46	a94	C8	d94
H95	C90	b95	C46	a95	C8	d95
H96	C91	b96	C46	a96	C8	d96
H97	C91	b97	C46	a97	C8	d97
H98	C91	b98	C46	a98	C8	d98
C99	C55	b99	C11	a99	P6	d99
C100	C55	b100	C11	a100	P6	d100
H101	C55	b101	C11	a101	P6	d101
H102	C99	b102	C55	a102	C11	d102
H103	C99	b103	C55	a103	C11	d103
H104	C99	b104	C55	a104	C11	d104
H105	C100	b105	C55	a105	C11	d105
H106	C100	b106	C55	a106	C11	d106
H107	C100	b107	C55	a107	C11	d107
C108	C58	b108	C12	a108	P6	d108
C109	C58	b109	C12	a109	P6	d109
H110	C58	b110	C12	a110	P6	d110
H111	C108	b111	C58	a111	C12	d111
H112	C108	b112	C58	a112	C12	d112
H113	C108	b113	C58	a113	C12	d113
H114	C109	b114	C58	a114	C12	d114
H115	C109	b115	C58	a115	C12	d115
H116	C109	b116	C58	a116	C12	d116
C117	C48	b117	C9	a117	P4	d117
C118	C48	b118	C9	a118	P4	d118
H119	C48	b119	C9	a119	P4	d119
H120	C117	b120	C48	a120	C9	d120
H121	C117	b121	C48	a121	C9	d121
H122	C117	b122	C48	a122	C9	d122
H123	C118	b123	C48	a123	C9	d123
H124	C118	b124	C48	a124	C9	d124
H125	C118	b125	C48	a125	C9	d125
C126	C51	b126	C10	a126	P4	d126
C127	C51	b127	C10	a127	P4	d127
H128	C51	b128	C10	a128	P4	d128
H129	C126	b129	C51	a129	C10	d129
H130	C126	b130	C51	a130	C10	d130
H131	C126	b131	C51	a131	C10	d131
H132	C127	b132	C51	a132	C10	d132
H133	C127	b133	C51	a133	C10	d133
H134	C127	b134	C51	a134	C10	d134
C135	C60	b135	C13	a135	P3	d135
C136	C60	b136	C13	a136	P3	d136
H137	C60	b137	C13	a137	P3	d137
H138	C135	b138	C60	a138	C13	d138

H139	C135	b139	C60	a139	C13	d139
H140	C135	b140	C60	a140	C13	d140
H141	C136	b141	C60	a141	C13	d141
H142	C136	b142	C60	a142	C13	d142
H143	C136	b143	C60	a143	C13	d143
C144	C63	b144	C14	a144	P3	d144
C145	C63	b145	C14	a145	P3	d145
H146	C63	b146	C14	a146	P3	d146
H147	C144	b147	C63	a147	C14	d147
H148	C144	b148	C63	a148	C14	d148
H149	C144	b149	C63	a149	C14	d149
H150	C145	b150	C63	a150	C14	d150
H151	C145	b151	C63	a151	C14	d151
H152	C145	b152	C63	a152	C14	d152
C153	C66	b153	C19	a153	C18	d153
C154	C66	b154	C19	a154	C18	d154
C155	C66	b155	C19	a155	C18	d155
H156	C153	b156	C66	a156	C19	d156
H157	C153	b157	C66	a157	C19	d157
H158	C153	b158	C66	a158	C19	d158
H159	C154	b159	C66	a159	C19	d159
H160	C154	b160	C66	a160	C19	d160
H161	C154	b161	C66	a161	C19	d161
H162	C155	b162	C66	a162	C19	d162
H163	C155	b163	C66	a163	C19	d163
H164	C155	b164	C66	a164	C19	d164
C165	C71	b165	C26	a165	C25	d165
C166	C71	b166	C26	a166	C25	d166
C167	C71	b167	C26	a167	C25	d167
H168	C165	b168	C71	a168	C26	d168
H169	C165	b169	C71	a169	C26	d169
H170	C165	b170	C71	a170	C26	d170
H171	C166	b171	C71	a171	C26	d171
H172	C166	b172	C71	a172	C26	d172
H173	C166	b173	C71	a173	C26	d173
H174	C167	b174	C71	a174	C26	d174
H175	C167	b175	C71	a175	C26	d175
H176	C167	b176	C71	a176	C26	d176
C177	C73	b177	C29	a177	P3	d177
C178	C73	b178	C29	a178	P3	d178
C179	C73	b179	C29	a179	P3	d179
H180	C177	b180	C73	a180	C29	d180
H181	C177	b181	C73	a181	C29	d181
H182	C177	b182	C73	a182	C29	d182
H183	C178	b183	C73	a183	C29	d183
H184	C178	b184	C73	a184	C29	d184

H185	C178	b185	C73	a185	C29	d185
H186	C179	b186	C73	a186	C29	d186
H187	C179	b187	C73	a187	C29	d187
H188	C179	b188	C73	a188	C29	d188
C189	C80	b189	C40	a189	C39	d189
C190	C80	b190	C40	a190	C39	d190
C191	C80	b191	C40	a191	C39	d191
H192	C189	b192	C80	a192	C40	d192
H193	C189	b193	C80	a193	C40	d193
H194	C189	b194	C80	a194	C40	d194
H195	C190	b195	C80	a195	C40	d195
H196	C190	b196	C80	a196	C40	d196
H197	C190	b197	C80	a197	C40	d197
H198	C191	b198	C80	a198	C40	d198
H199	C191	b199	C80	a199	C40	d199
H200	C191	b200	C80	a200	C40	d200

\$

\$zvar

b2 =	2.8103572613		
b3 =	2.3023920350	a3 =	111.4876965378
b4 =	2.3015364335	a4 =	111.5685636817
b5 =	2.3120180405	a5 =	109.7465520150
b6 =	2.3129592623	a6 =	109.9798568021
b7 =	1.9025676654	a7 =	122.7330159707
b8 =	1.9028562478	a8 =	118.5070210360
b9 =	1.9093135018	a9 =	116.8126226898
b10 =	1.8938320856	a10 =	123.8644784677
b11 =	1.9024183876	a11 =	122.6456541218
b12 =	1.9025095199	a12 =	118.6244468264
b13 =	1.9093674645	a13 =	116.9192870593
b14 =	1.8939197083	a14 =	123.7326487148
b15 =	2.2159139762	a15 =	50.6593953512
b16 =	2.2090474921	a16 =	50.4801256233
b17 =	1.8578676979	a17 =	99.0586467137
b18 =	1.4099704855	a18 =	122.2756871335
b19 =	1.3934200773	a19 =	123.0625185001
b20 =	1.4071905118	a20 =	116.4486917125
b21 =	1.3820962391	a21 =	121.6703316409
b22 =	1.4176622102	a22 =	122.3330441677
b23 =	1.4186928600	a23 =	117.9397906901
b24 =	1.4175336034	a24 =	119.8934496702
b25 =	1.3821545756	a25 =	122.3537050620
b26 =	1.4073783065	a26 =	121.6191722145
b27 =	1.3931332451	a27 =	116.4937291273
b28 =	1.4101489551	a28 =	123.0577602877
b29 =	4.1832942576	a29 =	115.9996802242

d4 =	-129.9244491447
d5 =	47.7094182796
d6 =	177.4587239748
d7 =	149.5667139170
d8 =	-74.3038825138
d9 =	145.4594683684
d10 =	-78.7583949648
d11 =	148.7749877263
d12 =	-75.0422910035
d13 =	145.8725882317
d14 =	-78.2360017679
d15 =	65.0163972629
d16 =	-115.3003441973
d17 =	40.6849091403
d18 =	179.9265807050
d19 =	-174.6194716245
d20 =	-0.3831916477
d21 =	0.7071095773
d22 =	0.1171907948
d23 =	110.4675583082
d24 =	90.4068448621
d25 =	178.1463161775
d26 =	0.2102145857
d27 =	0.6029404671
d28 =	-0.3608408567
d29 =	35.8263923588

b30 =	1.3943152214	a30 =	16.7230602022	d30 =	-159.1952784904
b31 =	1.4097366220	a31 =	122.8382948545	d31 =	9.6149768623
b32 =	1.4172976473	a32 =	120.0622334160	d32 =	1.9167346795
b33 =	1.4165698569	a33 =	116.6415793259	d33 =	-1.2180370770
b34 =	1.3821030982	a34 =	122.1307590095	d34 =	-0.1340022381
b35 =	3.7324261243	a35 =	114.2344901529	d35 =	132.4188213703
b36 =	1.3821139410	a36 =	17.9660893709	d36 =	80.0637529667
b37 =	1.4165985539	a37 =	122.1357214920	d37 =	0.9335652224
b38 =	1.4174310763	a38 =	116.6681068025	d38 =	-0.2762281518
b39 =	1.4099473328	a39 =	120.0329434356	d39 =	-1.1860595927
b40 =	1.3947598634	a40 =	122.8323066904	d40 =	2.1003735043
b41 =	1.1021672290	a41 =	104.5055120140	d41 =	-38.0476116687
b42 =	1.0970789462	a42 =	108.3829806553	d42 =	-151.9305036663
b43 =	1.5462704223	a43 =	116.9336675774	d43 =	83.0648278177
b44 =	1.0989274120	a44 =	102.0187545722	d44 =	31.1684179916
b45 =	1.1027208500	a45 =	104.4854058701	d45 =	-78.9366101939
b46 =	1.5508052621	a46 =	124.8106942919	d46 =	154.3348338313
b47 =	1.1003751947	a47 =	101.5449803935	d47 =	-29.2372483275
b48 =	1.5492362183	a48 =	123.9805979990	d48 =	-150.6318347426
b49 =	1.1017299760	a49 =	105.6796972302	d49 =	81.5029881180
b50 =	1.1013032936	a50 =	104.4920815292	d50 =	33.4674771450
b51 =	1.5497058351	a51 =	116.3306141839	d51 =	-87.1837313326
b52 =	1.0978780194	a52 =	109.4146396553	d52 =	148.4700624605
b53 =	1.1021697788	a53 =	104.5258228508	d53 =	-38.1444855710
b54 =	1.0970021344	a54 =	108.3746450589	d54 =	-152.0428170364
b55 =	1.5464814911	a55 =	116.8668974190	d55 =	82.9568073140
b56 =	1.0988709134	a56 =	101.9831055000	d56 =	31.3083941272
b57 =	1.1026795099	a57 =	104.4737479100	d57 =	-78.8174282795
b58 =	1.5507612082	a58 =	124.8490113589	d58 =	154.4509984118
b59 =	1.1003814813	a59 =	101.5299813887	d59 =	-29.3826069956
b60 =	1.5492342571	a60 =	123.9860385959	d60 =	-150.7556874934
b61 =	1.1016789171	a61 =	105.7120957216	d61 =	81.3702179563
b62 =	1.1012969150	a62 =	104.4943369441	d62 =	33.6700016095
b63 =	1.5494715591	a63 =	116.3212884160	d63 =	-86.9142826482
b64 =	1.0979161341	a64 =	109.3961063060	d64 =	148.6706687620
b65 =	1.0842147187	a65 =	118.1761665630	d65 =	3.0082223771
b66 =	1.5352123646	a66 =	123.3814554346	d66 =	177.8058649807
b67 =	1.0893157399	a67 =	119.9087117755	d67 =	-179.9124610828
b68 =	1.0873295695	a68 =	119.3941863259	d68 =	179.2872483802
b69 =	1.0873099129	a69 =	118.2535900542	d69 =	-1.0812003757
b70 =	1.0891062753	a70 =	118.4579420322	d70 =	-179.2976555971
b71 =	1.5350299606	a71 =	120.1183538860	d71 =	-177.9975968717
b72 =	1.0843075635	a72 =	118.7048100301	d72 =	-178.0186877437
b73 =	1.5358069007	a73 =	139.5627090298	d73 =	-175.9314762383
b74 =	1.0855987829	a74 =	118.8361706993	d74 =	-168.7591560228
b75 =	1.0878275586	a75 =	118.2537975904	d75 =	-179.8923055050

b76 =	1.0892689150	a76 =	118.4400355110	d76 =	-179.3513381470
b77 =	1.0889761148	a77 =	136.4133438231	d77 =	79.8913123836
b78 =	1.0877879768	a78 =	119.6197380190	d78 =	-179.3637103997
b79 =	1.0858112364	a79 =	118.2781662188	d79 =	-179.7584609974
b80 =	1.5356673928	a80 =	123.3680519580	d80 =	176.1136175594
b81 =	1.5460909268	a81 =	109.9626340388	d81 =	172.1306133448
b82 =	1.5403591847	a82 =	111.7812565284	d82 =	-64.9366759927
b83 =	1.0990922569	a83 =	108.7493961516	d83 =	54.6482316580
b84 =	1.1000965534	a84 =	110.6901112160	d84 =	-179.3392991085
b85 =	1.0999137658	a85 =	111.2183978802	d85 =	-59.2483170658
b86 =	1.1014322723	a86 =	110.5943801266	d86 =	60.9764024332
b87 =	1.1016721180	a87 =	110.1161318317	d87 =	-65.0440994174
b88 =	1.0973055856	a88 =	111.3056834698	d88 =	54.4517466394
b89 =	1.0996181310	a89 =	110.6840372622	d89 =	175.5138467404
b90 =	1.5436689979	a90 =	113.9156514102	d90 =	72.9770052205
b91 =	1.5484839451	a91 =	108.9350958819	d91 =	-165.3691403233
b92 =	1.0969458012	a92 =	108.7708970575	d92 =	-48.5848016006
b93 =	1.1002152129	a93 =	110.1588389334	d93 =	176.7026747354
b94 =	1.0961977444	a94 =	112.6499057931	d94 =	-63.0084470918
b95 =	1.1012875417	a95 =	110.3878577012	d95 =	57.9136247535
b96 =	1.1013991885	a96 =	110.5992356572	d96 =	-62.1657455554
b97 =	1.0983173138	a97 =	111.2625608481	d97 =	57.7178973874
b98 =	1.1000503940	a98 =	110.5068926265	d98 =	178.3224085068
b99 =	1.5457624430	a99 =	109.9859179194	d99 =	171.9833896848
b100 =	1.5402130987	a100 =	111.7149875130	d100 =	-65.0808459769
b101 =	1.0989997719	a101 =	108.7420101245	d101 =	54.4801702877
b102 =	1.1000790480	a102 =	110.7094613399	d102 =	-179.4462934072
b103 =	1.0998995510	a103 =	111.2032050990	d103 =	-59.3439067602
b104 =	1.1014131324	a104 =	110.5753189059	d104 =	60.8709061610
b105 =	1.1016854781	a105 =	110.0959264991	d105 =	-65.5009871539
b106 =	1.0972452467	a106 =	111.2461228313	d106 =	53.9362968545
b107 =	1.0996189475	a107 =	110.7326766188	d107 =	175.0364065221
b108 =	1.5438679037	a108 =	113.9166129600	d108 =	72.7795086616
b109 =	1.5485048261	a109 =	108.9424334184	d109 =	-165.5503513821
b110 =	1.0968636568	a110 =	108.7913601108	d110 =	-48.8211458013
b111 =	1.1002175883	a111 =	110.1568977972	d111 =	176.6919819768
b112 =	1.0961620998	a112 =	112.6302726264	d112 =	-63.0159668429
b113 =	1.1013086646	a113 =	110.3887920419	d113 =	57.8867060469
b114 =	1.1014188427	a114 =	110.6179946786	d114 =	-62.3846904974
b115 =	1.0983225274	a115 =	111.2451481851	d115 =	57.5080928669
b116 =	1.1000735292	a116 =	110.4866577395	d116 =	178.1095869267
b117 =	1.5496524539	a117 =	108.9521949962	d117 =	162.6544183685
b118 =	1.5428969618	a118 =	113.6601691323	d118 =	-75.5272538120
b119 =	1.0973491903	a119 =	108.6090035587	d119 =	45.5458043261
b120 =	1.1000268671	a120 =	110.5993769039	d120 =	-178.9871720619
b121 =	1.0995014393	a121 =	111.2827987093	d121 =	-58.8539738511

b122=	1.1017024626	a122=	110.6673018192	d122=	61.4725280823
b123=	1.1013429748	a123=	110.5036458412	d123=	-59.3151188021
b124=	1.0966848365	a124=	112.3666146433	d124=	61.5750594754
b125=	1.1002446710	a125=	110.1624059561	d125=	-178.1492147445
b126=	1.5412939887	a126=	112.9527424487	d126=	57.0661840789
b127=	1.5462240966	a127=	109.4934234296	d127=	-179.7517876470
b128=	1.0986698442	a128=	108.3454423935	d128=	-62.8943377558
b129=	1.1003391074	a129=	110.0707091736	d129=	179.5182501452
b130=	1.0985788060	a130=	111.6983356820	d130=	-60.3518999188
b131=	1.0988275635	a131=	110.5817009518	d131=	59.6154767956
b132=	1.1009164494	a132=	110.6206932939	d132=	-63.6239693935
b133=	1.1001501732	a133=	111.1931360030	d133=	56.9135728079
b134=	1.0999731934	a134=	110.5215249046	d134=	176.7991021410
b135=	1.5495797290	a135=	108.9663386343	d135=	162.5060802247
b136=	1.5429172702	a136=	113.6419375506	d136=	-75.6535161713
b137=	1.0972105773	a137=	108.6349978938	d137=	45.4362162096
b138=	1.1000547202	a138=	110.5964276483	d138=	-179.0740901495
b139=	1.0995301617	a139=	111.2687986765	d139=	-58.9608998218
b140=	1.1016836751	a140=	110.6829959030	d140=	61.3726335722
b141=	1.1013411521	a141=	110.5003434927	d141=	-59.3908615868
b142=	1.0967075189	a142=	112.3571102629	d142=	61.4784282417
b143=	1.1002380960	a143=	110.1656902218	d143=	-178.2371418018
b144=	1.5415662405	a144=	112.9209192507	d144=	57.6334311959
b145=	1.5464401074	a145=	109.5331033487	d145=	-179.2150414676
b146=	1.0987325284	a146=	108.3776715151	d146=	-62.3358196564
b147=	1.1003718956	a147=	110.0452081125	d147=	179.7040327615
b148=	1.0985802716	a148=	111.7204154952	d148=	-60.1677033834
b149=	1.0988298088	a149=	110.6463733058	d149=	59.7980228014
b150=	1.1009890183	a150=	110.6329079687	d150=	-63.7151840267
b151=	1.1001474353	a151=	111.2202670231	d151=	56.8473928381
b152=	1.0999679214	a152=	110.5009857527	d152=	176.7346720595
b153=	1.5558258859	a153=	109.5745090414	d153=	-115.5173665101
b154=	1.5456143078	a154=	112.6282658672	d154=	4.5767093406
b155=	1.5539792875	a155=	110.1232606214	d155=	125.0931959616
b156=	1.1009145836	a156=	110.1664086780	d156=	-179.0649404526
b157=	1.0985950699	a157=	111.2504778833	d157=	-59.1963400423
b158=	1.0994543529	a158=	110.5859094226	d158=	61.0821362299
b159=	1.0999456340	a159=	109.3148821519	d159=	178.7746811613
b160=	1.0993943379	a160=	111.5428269931	d160=	-62.3509995469
b161=	1.0996271032	a161=	111.5148552364	d161=	59.5377046961
b162=	1.1007910705	a162=	110.0340567160	d162=	-179.0965104537
b163=	1.0995370106	a163=	110.7046422654	d163=	-59.1062082893
b164=	1.0983984712	a164=	111.4321377148	d164=	61.3041861581
b165=	1.5555356551	a165=	109.6658033969	d165=	61.5586860422
b166=	1.5457433188	a166=	112.6802816326	d166=	-178.2929932815
b167=	1.5540543370	a167=	109.9935945487	d167=	-57.8183982807

b168=	1.1008522999	a168=	110.1166484063	d168=	-179.0105012532
b169=	1.0985434262	a169=	111.2857389695	d169=	-59.1737662919
b170=	1.0994388480	a170=	110.5977444231	d170=	61.1479844920
b171=	1.0999357767	a171=	109.2834937226	d171=	179.0350191997
b172=	1.0994380757	a172=	111.5240500690	d172=	-62.0809529476
b173=	1.0996020738	a173=	111.5446825399	d173=	59.8346072244
b174=	1.1008372175	a174=	110.0657727479	d174=	-179.3799762214
b175=	1.0996077657	a175=	110.6789959809	d175=	-59.3806093178
b176=	1.0984718409	a176=	111.3890405588	d176=	60.9627914677
b177=	1.5561031867	a177=	109.3855136962	d177=	-108.6894629777
b178=	1.5458060535	a178=	112.6674873199	d178=	11.2904804636
b179=	1.5541007911	a179=	110.3999998196	d179=	132.0074984952
b180=	1.1008521236	a180=	110.1053282272	d180=	-179.3560303578
b181=	1.0986177211	a181=	111.2374554543	d181=	-59.5250407567
b182=	1.0995220458	a182=	110.6445266792	d182=	60.7821957857
b183=	1.0999040160	a183=	109.2694874860	d183=	179.0577005742
b184=	1.0993948188	a184=	111.6031160974	d184=	-62.0355450452
b185=	1.0994945970	a185=	111.4571672704	d185=	59.9377185725
b186=	1.1008309775	a186=	109.8697154455	d186=	179.7181448490
b187=	1.0990077777	a187=	110.7679221245	d187=	-60.4353428504
b188=	1.0983761335	a188=	111.4589219306	d188=	60.2596701810
b189=	1.5563356726	a189=	109.2549762184	d189=	-113.6939735699
b190=	1.5458948325	a190=	112.6958799658	d190=	6.2289654480
b191=	1.5539078460	a191=	110.4440387064	d191=	127.0174955084
b192=	1.1009000032	a192=	110.1596945447	d192=	-179.2695747318
b193=	1.0986649458	a193=	111.1927884709	d193=	-59.4010486852
b194=	1.0995501803	a194=	110.6303838216	d194=	60.8591877548
b195=	1.0999012227	a195=	109.2619302044	d195=	179.0456330172
b196=	1.0993328002	a196=	111.6284750084	d196=	-62.0606984467
b197=	1.0995118313	a197=	111.4569961742	d197=	59.9202336572
b198=	1.1008424436	a198=	109.8851938176	d198=	179.6964092321
b199=	1.0988954060	a199=	110.7728718112	d199=	-60.4511592126
b200=	1.0983337348	a200=	111.4654162067	d200=	60.2424758724

\$

&atomic

atom basis

CU1 lacv3p

CU2 lacv3p

&

Triplet state geometries were optimized using the Jaguar program with the following keywords, starting from the optimized ground state geometry:

dftname=b3lyp basis=midix igeopt=1 maxitg=30 iacscf=1 maxit=300 multip=3

And the following &atomic block:

```

&atomic
atom basis
CU1 lacv3p
CU2 lacv3p
&

```

The optimized geometry was then used in a single point calculation to obtain the triplet state energy with the following input file:

```

$gen
multip=3 dftname=b3lyp basis=midix igeopt=0
cut10=5.0e-4 cut20=5.0e-4 iuhf=1
$
$zmat
CU1
CU2  CU1  b2
P3   CU2  b3   CU1  a3
P4   CU1  b4   CU2  a4   P3   d4
P5   CU1  b5   CU2  a5   P3   d5
P6   CU2  b6   CU1  a6   P3   d6
C7   P5   b7   CU1  a7   CU2  d7
C8   P5   b8   CU1  a8   CU2  d8
C9   P4   b9   CU1  a9   CU2  d9
C10  P4   b10  CU1  a10  CU2  d10
C11  P6   b11  CU2  a11  CU1  d11
C12  P6   b12  CU2  a12  CU1  d12
C13  P3   b13  CU2  a13  CU1  d13
C14  P3   b14  CU2  a14  CU1  d14
N15  CU2  b15  CU1  a15  P3   d15
N16  CU2  b16  CU1  a16  P3   d16
C17  P6   b17  CU2  a17  CU1  d17
C18  C17  b18  P6   a18  CU2  d18
C19  C18  b19  C17  a19  P6   d19
C20  C19  b20  C18  a20  C17  d20
C21  C20  b21  C19  a21  C18  d21
C22  C21  b22  C20  a22  C19  d22
C23  N16  b23  CU2  a23  CU1  d23
C24  C23  b24  N16  a24  CU2  d24
C25  C24  b25  C23  a25  N16  d25
C26  C25  b26  C24  a26  C23  d26
C27  C26  b27  C25  a27  C24  d27
C28  C27  b28  C26  a28  C25  d28
C29  P3   b29  CU2  a29  CU1  d29
C30  C29  b30  P3   a30  CU2  d30
C31  C30  b31  C29  a31  P3   d31
C32  C31  b32  C30  a32  C29  d32

```

C33	C32	b33	C31	a33	C30	d33
C34	C33	b34	C32	a34	C31	d34
C35	N15	b35	CU2	a35	CU1	d35
C36	C35	b36	N15	a36	CU2	d36
C37	C36	b37	C35	a37	N15	d37
C38	C37	b38	C36	a38	C35	d38
C39	C38	b39	C37	a39	C36	d39
C40	C39	b40	C38	a40	C37	d40
H41	C7	b41	P5	a41	CU1	d41
H42	C7	b42	P5	a42	CU1	d42
C43	C7	b43	P5	a43	CU1	d43
H44	C8	b44	P5	a44	CU1	d44
H45	C8	b45	P5	a45	CU1	d45
C46	C8	b46	P5	a46	CU1	d46
H47	C9	b47	P4	a47	CU1	d47
C48	C9	b48	P4	a48	CU1	d48
H49	C9	b49	P4	a49	CU1	d49
H50	C10	b50	P4	a50	CU1	d50
C51	C10	b51	P4	a51	CU1	d51
H52	C10	b52	P4	a52	CU1	d52
H53	C11	b53	P6	a53	CU2	d53
H54	C11	b54	P6	a54	CU2	d54
C55	C11	b55	P6	a55	CU2	d55
H56	C12	b56	P6	a56	CU2	d56
H57	C12	b57	P6	a57	CU2	d57
C58	C12	b58	P6	a58	CU2	d58
H59	C13	b59	P3	a59	CU2	d59
C60	C13	b60	P3	a60	CU2	d60
H61	C13	b61	P3	a61	CU2	d61
H62	C14	b62	P3	a62	CU2	d62
C63	C14	b63	P3	a63	CU2	d63
H64	C14	b64	P3	a64	CU2	d64
H65	C18	b65	C17	a65	P6	d65
C66	C19	b66	C18	a66	C17	d66
H67	C20	b67	C19	a67	C18	d67
H68	C21	b68	C20	a68	C19	d68
H69	C24	b69	C23	a69	N16	d69
H70	C25	b70	C24	a70	C23	d70
C71	C26	b71	C25	a71	C24	d71
H72	C27	b72	C26	a72	C25	d72
C73	C29	b73	P3	a73	CU2	d73
H74	C30	b74	C29	a74	P3	d74
H75	C33	b75	C32	a75	C31	d75
H76	C34	b76	C33	a76	C32	d76
H77	C35	b77	N15	a77	CU2	d77
H78	C36	b78	C35	a78	N15	d78

H79	C39	b79	C38	a79	C37	d79
C80	C40	b80	C39	a80	C38	d80
C81	C43	b81	C7	a81	P5	d81
C82	C43	b82	C7	a82	P5	d82
H83	C43	b83	C7	a83	P5	d83
H84	C81	b84	C43	a84	C7	d84
H85	C81	b85	C43	a85	C7	d85
H86	C81	b86	C43	a86	C7	d86
H87	C82	b87	C43	a87	C7	d87
H88	C82	b88	C43	a88	C7	d88
H89	C82	b89	C43	a89	C7	d89
C90	C46	b90	C8	a90	P5	d90
C91	C46	b91	C8	a91	P5	d91
H92	C46	b92	C8	a92	P5	d92
H93	C90	b93	C46	a93	C8	d93
H94	C90	b94	C46	a94	C8	d94
H95	C90	b95	C46	a95	C8	d95
H96	C91	b96	C46	a96	C8	d96
H97	C91	b97	C46	a97	C8	d97
H98	C91	b98	C46	a98	C8	d98
C99	C55	b99	C11	a99	P6	d99
C100	C55	b100	C11	a100	P6	d100
H101	C55	b101	C11	a101	P6	d101
H102	C99	b102	C55	a102	C11	d102
H103	C99	b103	C55	a103	C11	d103
H104	C99	b104	C55	a104	C11	d104
H105	C100	b105	C55	a105	C11	d105
H106	C100	b106	C55	a106	C11	d106
H107	C100	b107	C55	a107	C11	d107
C108	C58	b108	C12	a108	P6	d108
C109	C58	b109	C12	a109	P6	d109
H110	C58	b110	C12	a110	P6	d110
H111	C108	b111	C58	a111	C12	d111
H112	C108	b112	C58	a112	C12	d112
H113	C108	b113	C58	a113	C12	d113
H114	C109	b114	C58	a114	C12	d114
H115	C109	b115	C58	a115	C12	d115
H116	C109	b116	C58	a116	C12	d116
C117	C48	b117	C9	a117	P4	d117
C118	C48	b118	C9	a118	P4	d118
H119	C48	b119	C9	a119	P4	d119
H120	C117	b120	C48	a120	C9	d120
H121	C117	b121	C48	a121	C9	d121
H122	C117	b122	C48	a122	C9	d122
H123	C118	b123	C48	a123	C9	d123
H124	C118	b124	C48	a124	C9	d124

H125	C118	b125	C48	a125	C9	d125
C126	C51	b126	C10	a126	P4	d126
C127	C51	b127	C10	a127	P4	d127
H128	C51	b128	C10	a128	P4	d128
H129	C126	b129	C51	a129	C10	d129
H130	C126	b130	C51	a130	C10	d130
H131	C126	b131	C51	a131	C10	d131
H132	C127	b132	C51	a132	C10	d132
H133	C127	b133	C51	a133	C10	d133
H134	C127	b134	C51	a134	C10	d134
C135	C60	b135	C13	a135	P3	d135
C136	C60	b136	C13	a136	P3	d136
H137	C60	b137	C13	a137	P3	d137
H138	C135	b138	C60	a138	C13	d138
H139	C135	b139	C60	a139	C13	d139
H140	C135	b140	C60	a140	C13	d140
H141	C136	b141	C60	a141	C13	d141
H142	C136	b142	C60	a142	C13	d142
H143	C136	b143	C60	a143	C13	d143
C144	C63	b144	C14	a144	P3	d144
C145	C63	b145	C14	a145	P3	d145
H146	C63	b146	C14	a146	P3	d146
H147	C144	b147	C63	a147	C14	d147
H148	C144	b148	C63	a148	C14	d148
H149	C144	b149	C63	a149	C14	d149
H150	C145	b150	C63	a150	C14	d150
H151	C145	b151	C63	a151	C14	d151
H152	C145	b152	C63	a152	C14	d152
C153	C66	b153	C19	a153	C18	d153
C154	C66	b154	C19	a154	C18	d154
C155	C66	b155	C19	a155	C18	d155
H156	C153	b156	C66	a156	C19	d156
H157	C153	b157	C66	a157	C19	d157
H158	C153	b158	C66	a158	C19	d158
H159	C154	b159	C66	a159	C19	d159
H160	C154	b160	C66	a160	C19	d160
H161	C154	b161	C66	a161	C19	d161
H162	C155	b162	C66	a162	C19	d162
H163	C155	b163	C66	a163	C19	d163
H164	C155	b164	C66	a164	C19	d164
C165	C71	b165	C26	a165	C25	d165
C166	C71	b166	C26	a166	C25	d166
C167	C71	b167	C26	a167	C25	d167
H168	C165	b168	C71	a168	C26	d168
H169	C165	b169	C71	a169	C26	d169
H170	C165	b170	C71	a170	C26	d170

H171	C166	b171	C71	a171	C26	d171
H172	C166	b172	C71	a172	C26	d172
H173	C166	b173	C71	a173	C26	d173
H174	C167	b174	C71	a174	C26	d174
H175	C167	b175	C71	a175	C26	d175
H176	C167	b176	C71	a176	C26	d176
C177	C73	b177	C29	a177	P3	d177
C178	C73	b178	C29	a178	P3	d178
C179	C73	b179	C29	a179	P3	d179
H180	C177	b180	C73	a180	C29	d180
H181	C177	b181	C73	a181	C29	d181
H182	C177	b182	C73	a182	C29	d182
H183	C178	b183	C73	a183	C29	d183
H184	C178	b184	C73	a184	C29	d184
H185	C178	b185	C73	a185	C29	d185
H186	C179	b186	C73	a186	C29	d186
H187	C179	b187	C73	a187	C29	d187
H188	C179	b188	C73	a188	C29	d188
C189	C80	b189	C40	a189	C39	d189
C190	C80	b190	C40	a190	C39	d190
C191	C80	b191	C40	a191	C39	d191
H192	C189	b192	C80	a192	C40	d192
H193	C189	b193	C80	a193	C40	d193
H194	C189	b194	C80	a194	C40	d194
H195	C190	b195	C80	a195	C40	d195
H196	C190	b196	C80	a196	C40	d196
H197	C190	b197	C80	a197	C40	d197
H198	C191	b198	C80	a198	C40	d198
H199	C191	b199	C80	a199	C40	d199
H200	C191	b200	C80	a200	C40	d200

\$

\$zvar

b2 =	2.6281704140		
b3 =	2.3137819260	a3 =	111.7466342103
b4 =	2.3165436548	a4 =	111.5421549975
b5 =	2.3328702682	a5 =	110.3447967041
b6 =	2.3355008949	a6 =	110.0036127728
b7 =	1.9098555844	a7 =	120.5119894780
b8 =	1.9026425582	a8 =	119.9216315377
b9 =	1.9156199199	a9 =	115.4939826228
b10 =	1.8944480417	a10 =	123.8133938122
b11 =	1.9089877594	a11 =	120.4310921058
b12 =	1.9037772059	a12 =	120.2742686325
b13 =	1.9156225723	a13 =	115.5906682665
b14 =	1.8946052727	a14 =	123.5134641774
b15 =	2.1824418863	a15 =	52.7843667653
		d4 =	-130.3280260269
		d5 =	47.2002126796
		d6 =	177.2632412214
		d7 =	148.9079753762
		d8 =	-77.4561443610
		d9 =	146.8612788848
		d10 =	-79.8715228377
		d11 =	148.8716889794
		d12 =	-76.7808429756
		d13 =	146.5242815197
		d14 =	-80.6391980191
		d15 =	64.8633067764

b16 =	2.1664458087	a16 =	52.5545903893	d16 =	-114.8377141293
b17 =	1.8451865296	a17 =	98.7924931387	d17 =	41.5689418357
b18 =	1.4171507580	a18 =	122.9332098822	d18 =	-179.5950571656
b19 =	1.3911406347	a19 =	122.8471991848	d19 =	-174.7627114937
b20 =	1.4101095373	a20 =	117.1658530677	d20 =	-0.1997211112
b21 =	1.3875901670	a21 =	121.1921032698	d21 =	1.1478723932
b22 =	1.4099665171	a22 =	121.9019380165	d22 =	-0.3314075328
b23 =	1.4262742569	a23 =	117.7043049958	d23 =	110.5445042337
b24 =	1.4097808203	a24 =	119.9915230071	d24 =	92.6552418388
b25 =	1.3877178470	a25 =	121.8828013551	d25 =	178.3900435691
b26 =	1.4104396763	a26 =	121.1895751129	d26 =	-0.2993979186
b27 =	1.3909464440	a27 =	117.1789699582	d27 =	1.2665339372
b28 =	1.4171069718	a28 =	122.8314688109	d28 =	-0.5394350033
b29 =	4.1772230332	a29 =	115.8037328097	d29 =	35.3699877291
b30 =	1.3911873236	a30 =	17.6212711265	d30 =	-158.5910697680
b31 =	1.4199611441	a31 =	122.4880619268	d31 =	9.0722205930
b32 =	1.4213742257	a32 =	118.9685886516	d32 =	0.9894765803
b33 =	1.4058690245	a33 =	118.2879062324	d33 =	-0.2148533149
b34 =	1.3896868531	a34 =	121.5594175984	d34 =	-0.2543133548
b35 =	3.7336302699	a35 =	114.7000184010	d35 =	132.3197200715
b36 =	1.3895842355	a36 =	18.2198205241	d36 =	84.4170958686
b37 =	1.4059784904	a37 =	121.5323351435	d37 =	1.8134680364
b38 =	1.4217613713	a38 =	118.3021898981	d38 =	-0.2403162753
b39 =	1.4199764128	a39 =	118.9488707491	d39 =	-0.6652592911
b40 =	1.3912955414	a40 =	122.5106981795	d40 =	1.5830459163
b41 =	1.1021816440	a41 =	104.5966951436	d41 =	-35.5936538295
b42 =	1.0978187737	a42 =	107.2781955462	d42 =	-149.1584624992
b43 =	1.5449563295	a43 =	117.7236333775	d43 =	86.2024103829
b44 =	1.0984706866	a44 =	102.0948570282	d44 =	30.0519537737
b45 =	1.1023226089	a45 =	104.6237593533	d45 =	-80.5135632307
b46 =	1.5507307313	a46 =	124.6018195230	d46 =	152.7512310134
b47 =	1.0999117297	a47 =	101.7621016120	d47 =	-28.5826134155
b48 =	1.5491798405	a48 =	122.6902585458	d48 =	-149.4089111363
b49 =	1.1017051937	a49 =	106.4391753395	d49 =	82.7358430732
b50 =	1.1008964299	a50 =	104.5268427178	d50 =	33.0124848779
b51 =	1.5494712605	a51 =	116.5461001509	d51 =	-88.0919602193
b52 =	1.0980059528	a52 =	108.8382299072	d52 =	147.7569042122
b53 =	1.1022736004	a53 =	104.5273045927	d53 =	-35.4059907805
b54 =	1.0980798538	a54 =	107.3068749131	d54 =	-148.9118054661
b55 =	1.5456233497	a55 =	117.8137031607	d55 =	86.3668477611
b56 =	1.0986030361	a56 =	101.9949814444	d56 =	30.9592687577
b57 =	1.1027380068	a57 =	104.6512723784	d57 =	-79.5060985037
b58 =	1.5519605670	a58 =	124.6121041720	d58 =	153.7870023467
b59 =	1.0999286491	a59 =	101.6894609208	d59 =	-29.7348097067
b60 =	1.5497608489	a60 =	122.7800076916	d60 =	-150.3765500715
b61 =	1.1015687088	a61 =	106.4508751396	d61 =	81.5814778728

b62 =	1.1009097058	a62 =	104.5804231113	d62 =	34.1252377933
b63 =	1.5496350949	a63 =	116.2875583994	d63 =	-86.7819271514
b64 =	1.0980976611	a64 =	108.9023520937	d64 =	148.9480094725
b65 =	1.0836545587	a65 =	118.1733149596	d65 =	2.5055131574
b66 =	1.5354206855	a66 =	123.0991651915	d66 =	177.3603789152
b67 =	1.0883791659	a67 =	120.1271266893	d67 =	179.9231588713
b68 =	1.0870663743	a68 =	119.5411264523	d68 =	179.1022502263
b69 =	1.0871415339	a69 =	118.5911337839	d69 =	-1.0576223331
b70 =	1.0883698898	a70 =	118.6768264536	d70 =	-179.1422004803
b71 =	1.5350512458	a71 =	119.7619004981	d71 =	-176.7333883145
b72 =	1.0838910019	a72 =	118.9248503941	d72 =	-177.8515567152
b73 =	1.5354382265	a73 =	140.0747959166	d73 =	-175.2663828468
b74 =	1.0852131377	a74 =	119.1670920678	d74 =	-168.8298998842
b75 =	1.0875639345	a75 =	118.5806753169	d75 =	179.4762616479
b76 =	1.0879924173	a76 =	118.7850297670	d76 =	-179.4524801978
b77 =	1.0878702996	a77 =	136.9502065978	d77 =	83.1140330892
b78 =	1.0876118306	a78 =	119.8517118846	d78 =	-177.9219697636
b79 =	1.0853377204	a79 =	118.2582456845	d79 =	179.1818755391
b80 =	1.5361901232	a80 =	123.0510324204	d80 =	175.5734538634
b81 =	1.5470714972	a81 =	109.9327011671	d81 =	171.7257380607
b82 =	1.5403081856	a82 =	111.7356326886	d82 =	-65.3003131877
b83 =	1.0991025494	a83 =	108.7698429775	d83 =	54.2512792160
b84 =	1.1000195671	a84 =	110.6206598227	d84 =	-179.4309224759
b85 =	1.1002427743	a85 =	111.2338681557	d85 =	-59.3837853947
b86 =	1.1018349821	a86 =	110.6455692484	d86 =	60.9040319489
b87 =	1.1022019980	a87 =	110.1683455335	d87 =	-64.4742745218
b88 =	1.0979674176	a88 =	111.3757450769	d88 =	55.0758204648
b89 =	1.0996199762	a89 =	110.7334520661	d89 =	175.9933308919
b90 =	1.5440333991	a90 =	113.9404755200	d90 =	71.4584719485
b91 =	1.5494316287	a91 =	108.7287171865	d91 =	-167.0123124684
b92 =	1.0969548750	a92 =	108.6093424007	d92 =	-49.9667378016
b93 =	1.1000816677	a93 =	110.1095400799	d93 =	176.4246318446
b94 =	1.0967903156	a94 =	112.6103403524	d94 =	-63.3459265324
b95 =	1.1009493396	a95 =	110.5208765923	d95 =	57.6215523794
b96 =	1.1015772393	a96 =	110.4674318826	d96 =	-63.5013449435
b97 =	1.0985760986	a97 =	111.3468661387	d97 =	56.3125312883
b98 =	1.0997007724	a98 =	110.6219441220	d98 =	177.0445730505
b99 =	1.5464429436	a99 =	109.8396753403	d99 =	171.3497775025
b100 =	1.5398817589	a100 =	111.7626403180	d100 =	-65.7717723617
b101 =	1.0989486707	a101 =	108.8354725302	d101 =	53.9509994542
b102 =	1.1003321029	a102 =	110.6561538484	d102 =	-179.5141760229
b103 =	1.1002179260	a103 =	111.2026679506	d103 =	-59.4304913181
b104 =	1.1017554212	a104 =	110.5907605179	d104 =	60.7949091055
b105 =	1.1018144824	a105 =	110.1268188456	d105 =	-64.5678821713
b106 =	1.0976351656	a106 =	111.3790128853	d106 =	54.9842458299
b107 =	1.0999268889	a107 =	110.7430473728	d107 =	175.9056644617

b108=	1.5437919346	a108=	113.9404944508	d108=	72.6568553794
b109=	1.5483354625	a109=	108.9271703239	d109=	-165.7028586953
b110=	1.0967630252	a110=	108.7314669652	d110=	-48.8997426956
b111=	1.1002820396	a111=	110.1418784119	d111=	177.1393604453
b112=	1.0964180714	a112=	112.6296277916	d112=	-62.5997299653
b113=	1.1011039134	a113=	110.4068899780	d113=	58.3563331739
b114=	1.1014325578	a114=	110.6004178692	d114=	-62.5515597203
b115=	1.0983871917	a115=	111.2849355084	d115=	57.3095924784
b116=	1.1000452247	a116=	110.5036360073	d116=	177.9580933123
b117=	1.5496006139	a117=	108.9661098522	d117=	162.1303611230
b118=	1.5429191890	a118=	113.6319301474	d118=	-75.9754509766
b119=	1.0974672910	a119=	108.4814117835	d119=	44.9629856762
b120=	1.0999706837	a120=	110.5774881180	d120=	-178.9014255184
b121=	1.0994804795	a121=	111.3115591933	d121=	-58.8097692777
b122=	1.1016293018	a122=	110.6720516078	d122=	61.5380499044
b123=	1.1011966770	a123=	110.5516069055	d123=	-59.6949063729
b124=	1.0966331483	a124=	112.3278639633	d124=	61.2514501717
b125=	1.0999784163	a125=	110.1460211008	d125=	-178.5500838313
b126=	1.5411786085	a126=	112.8959105627	d126=	57.8599313412
b127=	1.5455567519	a127=	109.5318154950	d127=	-179.0304814666
b128=	1.0983248521	a128=	108.4023676121	d128=	-62.0574533837
b129=	1.1002461928	a129=	110.1141696801	d129=	-179.5026542464
b130=	1.0981532454	a130=	111.7528074539	d130=	-59.4325938949
b131=	1.0987652158	a131=	110.5902713869	d131=	60.6562650546
b132=	1.1005993525	a132=	110.6507424329	d132=	-63.3090973138
b133=	1.1000113301	a133=	111.1557023173	d133=	57.2166532028
b134=	1.0999728877	a134=	110.5069336451	d134=	177.0832279338
b135=	1.5495615899	a135=	108.9473038313	d135=	161.5030593320
b136=	1.5432068803	a136=	113.7312872137	d136=	-76.6183190280
b137=	1.0973093347	a137=	108.5163947329	d137=	44.3500503183
b138=	1.1000890131	a138=	110.5938034351	d138=	-179.2064003180
b139=	1.0995466677	a139=	111.2799164159	d139=	-59.0893040641
b140=	1.1016801903	a140=	110.6799618301	d140=	61.2438412892
b141=	1.1012531046	a141=	110.5460111461	d141=	-59.5408514862
b142=	1.0966244014	a142=	112.3332998159	d142=	61.4378804914
b143=	1.1001951617	a143=	110.1288191035	d143=	-178.3675314228
b144=	1.5417583916	a144=	112.7716453841	d144=	58.0369966775
b145=	1.5467525718	a145=	109.5968919367	d145=	-178.8960899289
b146=	1.0983038813	a146=	108.4518048829	d146=	-61.8049396070
b147=	1.1007089192	a147=	110.0869781509	d147=	-179.6788967634
b148=	1.0991965174	a148=	111.7733864360	d148=	-59.5558671580
b149=	1.0987213126	a149=	110.5380516817	d149=	60.5207197528
b150=	1.1007522219	a150=	110.6670075711	d150=	-63.0888131551
b151=	1.1003359936	a151=	111.2183682832	d151=	57.4500132355
b152=	1.1002553504	a152=	110.4885222992	d152=	177.3254349685
b153=	1.5561054136	a153=	109.3388724797	d153=	-115.1332695934

b154=	1.5459196210	a154=	112.7101256440	d154=	5.0718767889
b155=	1.5540862467	a155=	110.1134239874	d155=	125.6246930449
b156=	1.1010462036	a156=	110.1951792361	d156=	-179.1172946274
b157=	1.0984850679	a157=	111.3047356513	d157=	-59.1561926241
b158=	1.0996212241	a158=	110.4884509934	d158=	61.0405132493
b159=	1.0998804782	a159=	109.2882866758	d159=	179.0354233711
b160=	1.0994738724	a160=	111.6011415024	d160=	-62.0123774168
b161=	1.0996754552	a161=	111.4886228498	d161=	59.8570621454
b162=	1.1006951529	a162=	110.0036987297	d162=	-179.4473271363
b163=	1.0994332712	a163=	110.6447691787	d163=	-59.5730755140
b164=	1.0983135967	a164=	111.5273467252	d164=	60.8717612083
b165=	1.5561346671	a165=	109.5107199161	d165=	61.1725889845
b166=	1.5457394937	a166=	112.6825479267	d166=	-178.6103827901
b167=	1.5543612423	a167=	109.9610182060	d167=	-58.1238559626
b168=	1.1010562269	a168=	110.1143774195	d168=	-179.1492231551
b169=	1.0984353584	a169=	111.3465435842	d169=	-59.2296297931
b170=	1.0996531496	a170=	110.5547901456	d170=	61.0492223105
b171=	1.0998198144	a171=	109.2984237701	d171=	179.2417836785
b172=	1.0994418822	a172=	111.5791594080	d172=	-61.7976965665
b173=	1.0996274506	a173=	111.4994183097	d173=	60.0787114368
b174=	1.1007459015	a174=	110.0029169696	d174=	-179.4647346667
b175=	1.0994626100	a175=	110.6661346661	d175=	-59.5531974893
b176=	1.0983963956	a176=	111.4760695587	d176=	60.8237723505
b177=	1.5566902064	a177=	109.2125693943	d177=	-110.2324632264
b178=	1.5457974707	a178=	112.7175119832	d178=	9.8060120104
b179=	1.5541959169	a179=	110.1823069792	d179=	130.5214688732
b180=	1.1010943576	a180=	110.1179528478	d180=	-179.4550303425
b181=	1.0982923435	a181=	111.2635070001	d181=	-59.5155889945
b182=	1.0996533662	a182=	110.5418470437	d182=	60.7149449838
b183=	1.0999641299	a183=	109.3126538394	d183=	179.3512481957
b184=	1.0993623206	a184=	111.5558058303	d184=	-61.6613166373
b185=	1.0996173145	a185=	111.4288992684	d185=	60.2342178908
b186=	1.1009894397	a186=	109.8667725737	d186=	179.2351126496
b187=	1.0990301999	a187=	110.6786104240	d187=	-61.0082245210
b188=	1.0983406038	a188=	111.4962732550	d188=	59.6086314151
b189=	1.5560799701	a189=	109.0038706493	d189=	-113.0260173602
b190=	1.5461117353	a190=	113.0171215637	d190=	6.9446478360
b191=	1.5538434680	a191=	110.2993079438	d191=	127.8087895268
b192=	1.1010643620	a192=	110.1438291002	d192=	-179.0653302912
b193=	1.0985831400	a193=	111.2208121789	d193=	-59.0371167424
b194=	1.0995389155	a194=	110.5592208679	d194=	61.1457130766
b195=	1.0999310547	a195=	109.2749807679	d195=	179.3838530375
b196=	1.0990478128	a196=	111.6728990978	d196=	-61.6888380219
b197=	1.0991332275	a197=	111.4157508838	d197=	60.3105865266
b198=	1.1008590389	a198=	109.8073035772	d198=	179.5424556607
b199=	1.0986303954	a199=	110.7565256824	d199=	-60.7208587495

```

b200= 1.0982504625 a200= 111.5023199646 d200= 59.9743372322
$
&atomic
atom basis
CU1 lacv3p
CU2 lacv3p
&

```

The Gaussian TD-DFT calculations used ground state geometry from the Jaguar calculation and the following keywords:

```

b3lyp gen scf=(tight,direct) nofmm td=(50-50, nstates=8) pseudo=read

```

and the following basis set/pseudopotential block:

```

H C N P 0
midix
****
Cu 0
lanl2dz
****

```

```

Cu 0
lanl2dz

```